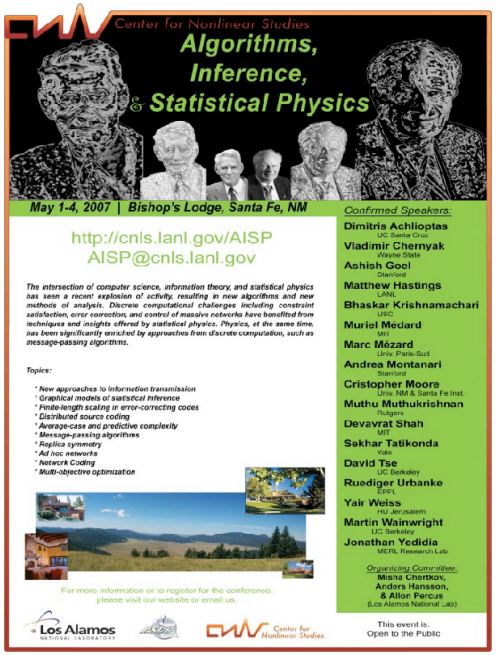
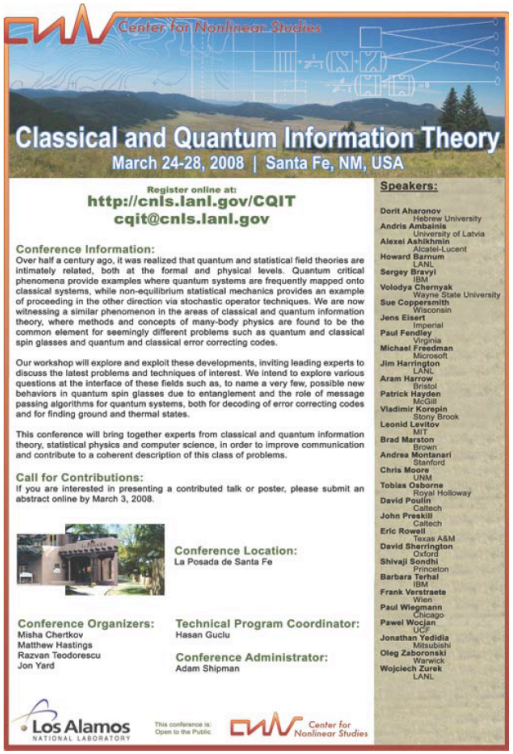
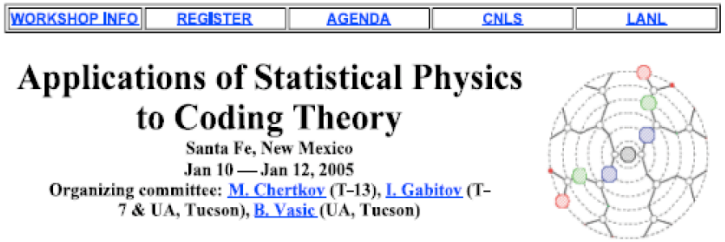
CNLS & Information Theory, Computer Science, Statistical Physics

- Conferences & Workshops **Series**







Los Alamos National Laboratory

a unique, irreplaceable national resource in the Department of Energy

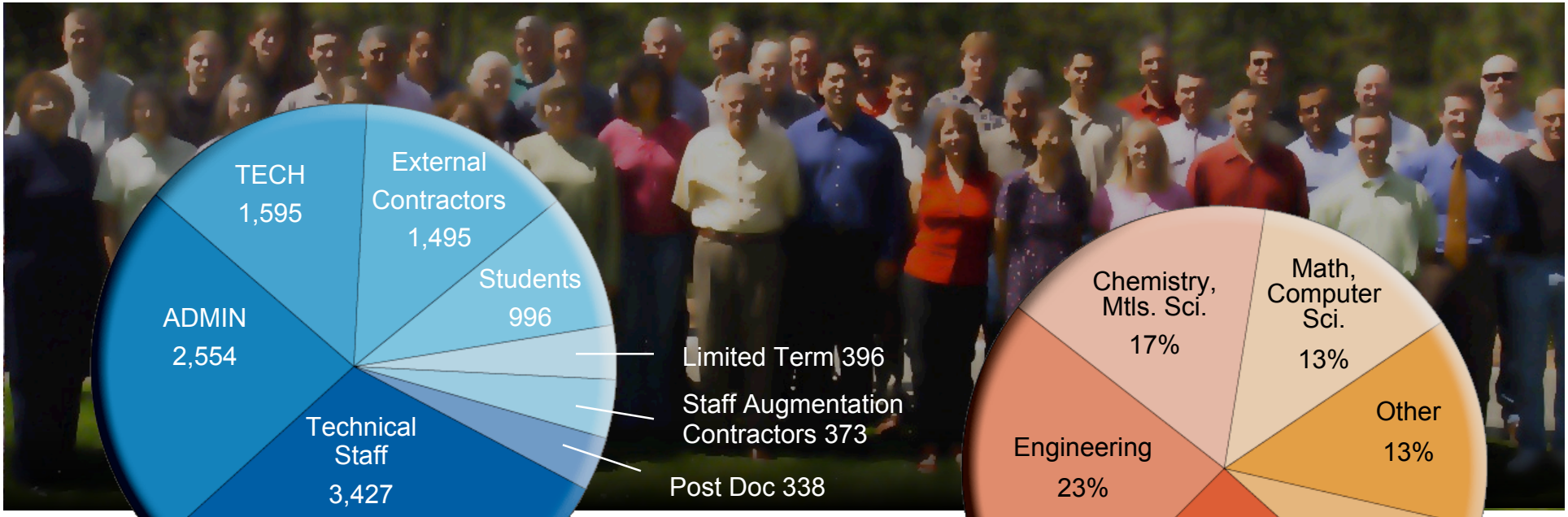
Los Alamos National Laboratory

- Is vital to the U.S.
- Is the most diverse scientific institution in the world
- Solves complex challenges that change society
- Develops revolutionary advances from national security to biomedical to climate and energy

Los Alamos
NATIONAL LABORATORY

DEPARTMENT OF ENERGY
UNITED STATES OF AMERICA

NNSA

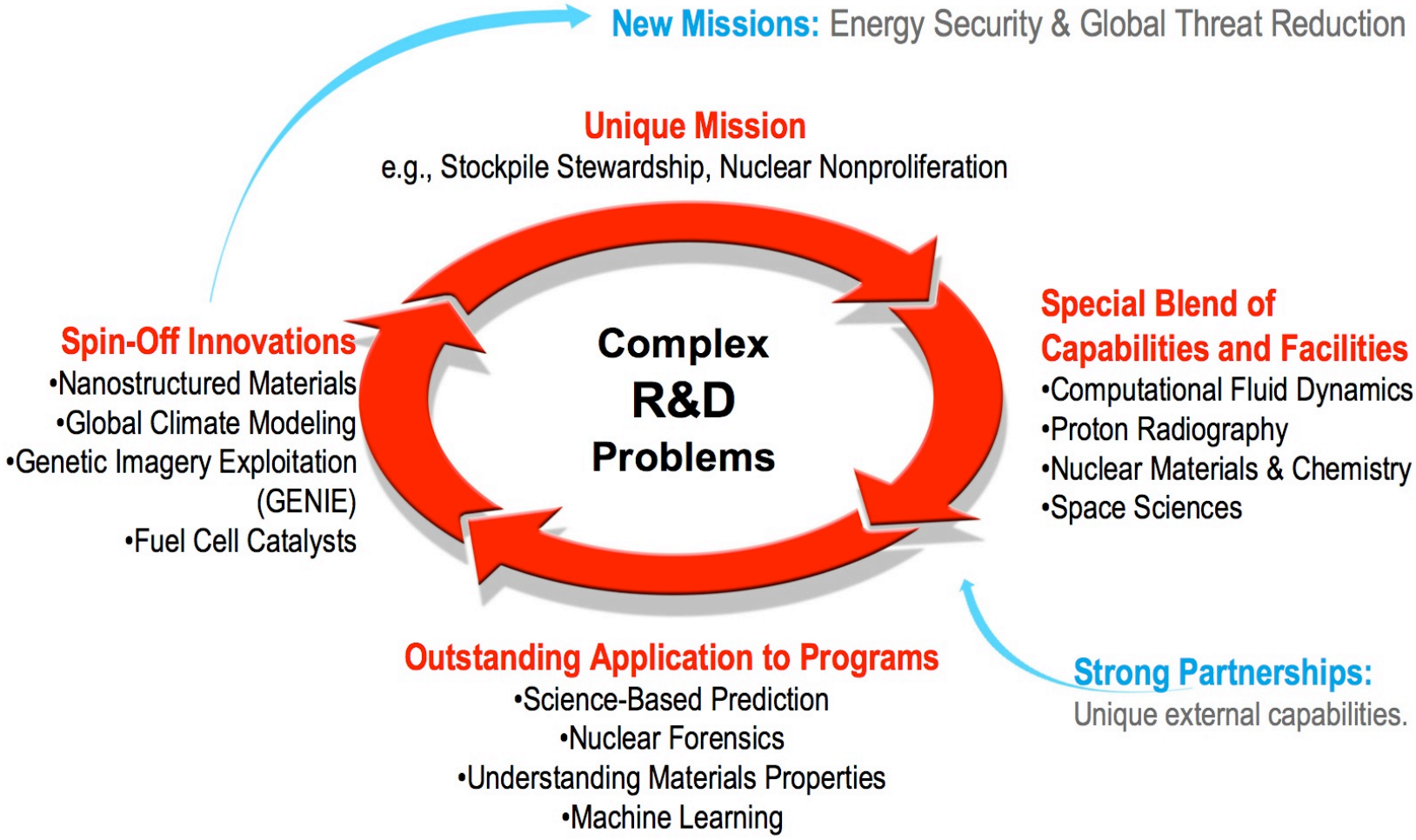


Technical Staff

LANL S&T base is Broad and Deep

- Drawn from across the nation
- 2,130 PhDs
- One quarter of workforce started as students or postdocs

Integrating capabilities, enables spin off innovations to tackle new challenges



National Security Science Laboratory: S,T&E Focus

Los Alamos is a material centric laboratory with unsurpassed nuclear and theory, modeling, and high-performance computing expertise and capabilities.

Forensic Science for Nuclear, Biological & Chemical Threats

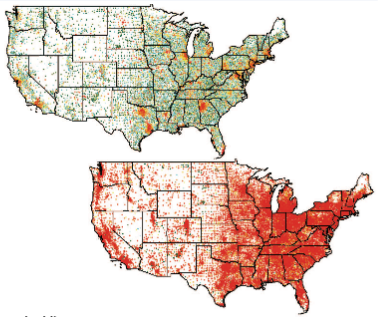
- Stewardship
- Weapons of Mass Destruction
- Energy

Information Science & Technology

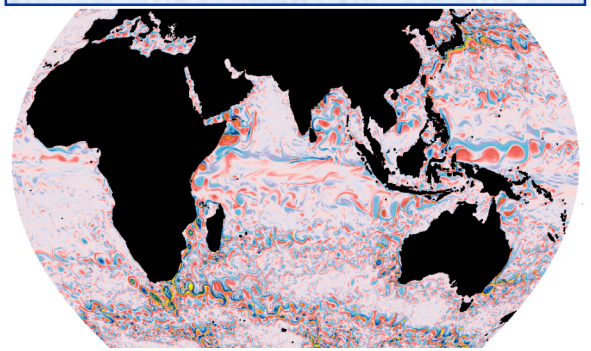
- Stewardship
- Data Sciences
- Intel
- Basic Science

Materials for the Future

- Detectors & Sensors
- Energy Science
- Materials for the Stockpile



Pandemic Modeling

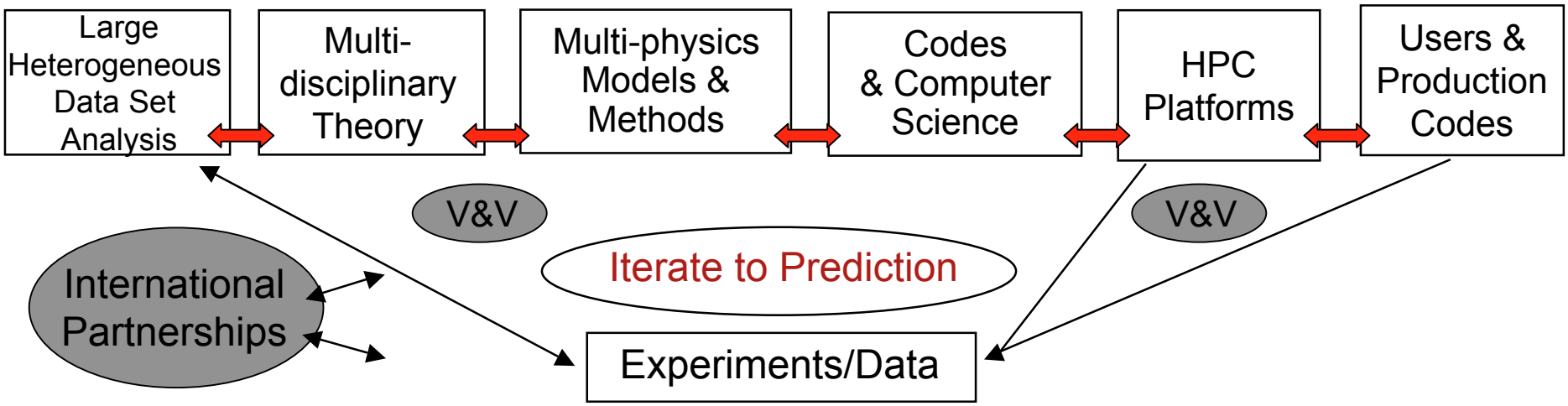


Ocean Vorticity Modeling

Soot Measurements

Theory, Modeling, Simulation and High-Performance Computing for Complex Systems

… LANL's Integration Capability … the heritage of 60+ years

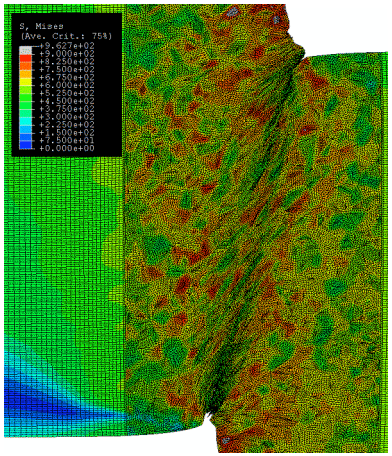


This integrated capability at scale is central to the huge national need for new generations of ideas, concepts, and methodologies to improve the fidelity, reliability, certainty, and usability of tools to guide and interpret experiments, and provide prediction and control for complex phenomena and systems.

Theory & models for simulations on HPC (petascale platforms for materials response)

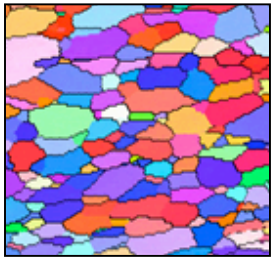
Macro-Mech.

Numerous constitutive models



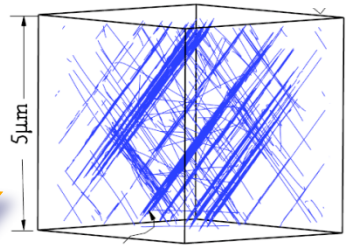
Polycrystal

Visco-plastic self consistent



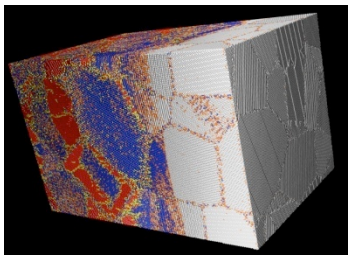
Single Crystal

G-L
Disl. Dyn. code



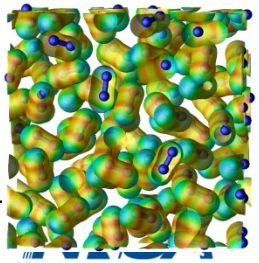
Molecular Dynamics

SPaSM
LAMMPS



Quantum Mechanics

VASP
MondoSCF



MaRIE

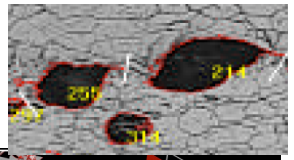
MaRIE data here

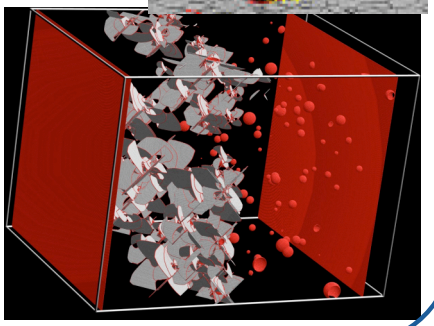
Example: Time evolution of ductile damage

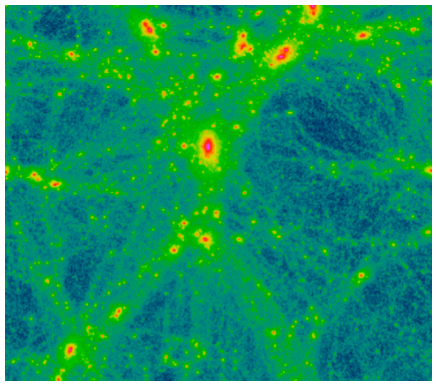
$\sim 10^{-3}\,\mu s \quad \mu s$

$\sim 20nm \quad 100\mu m$

Ta





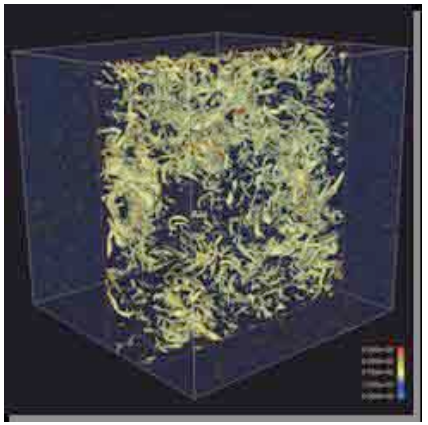


Cosmology: Filaments, Clusters, and Voids

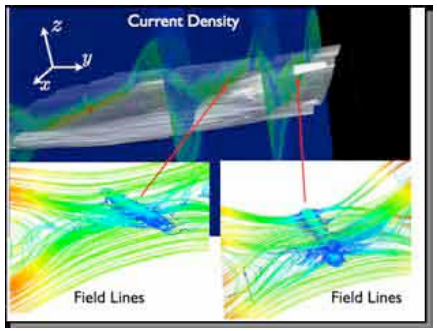
"The Century of Complexity"

(Systems of connected functional scales; Emergent properties)
Enabled by huge advances in Data, Simulation, Nonlinear Science…

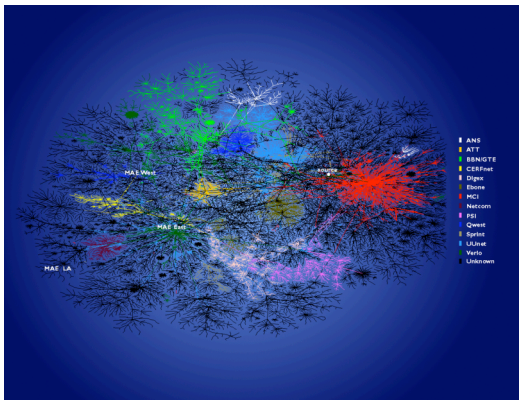
? Origins, Measures, Consequences ?



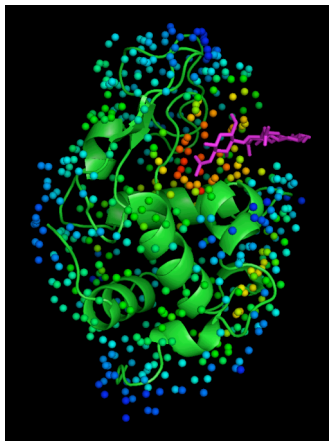
Fluid Turbulence



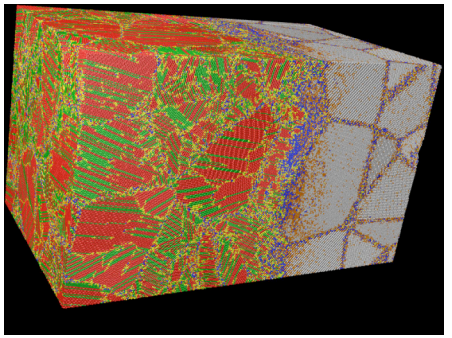
Magnetic Reconnection



Communication Networks



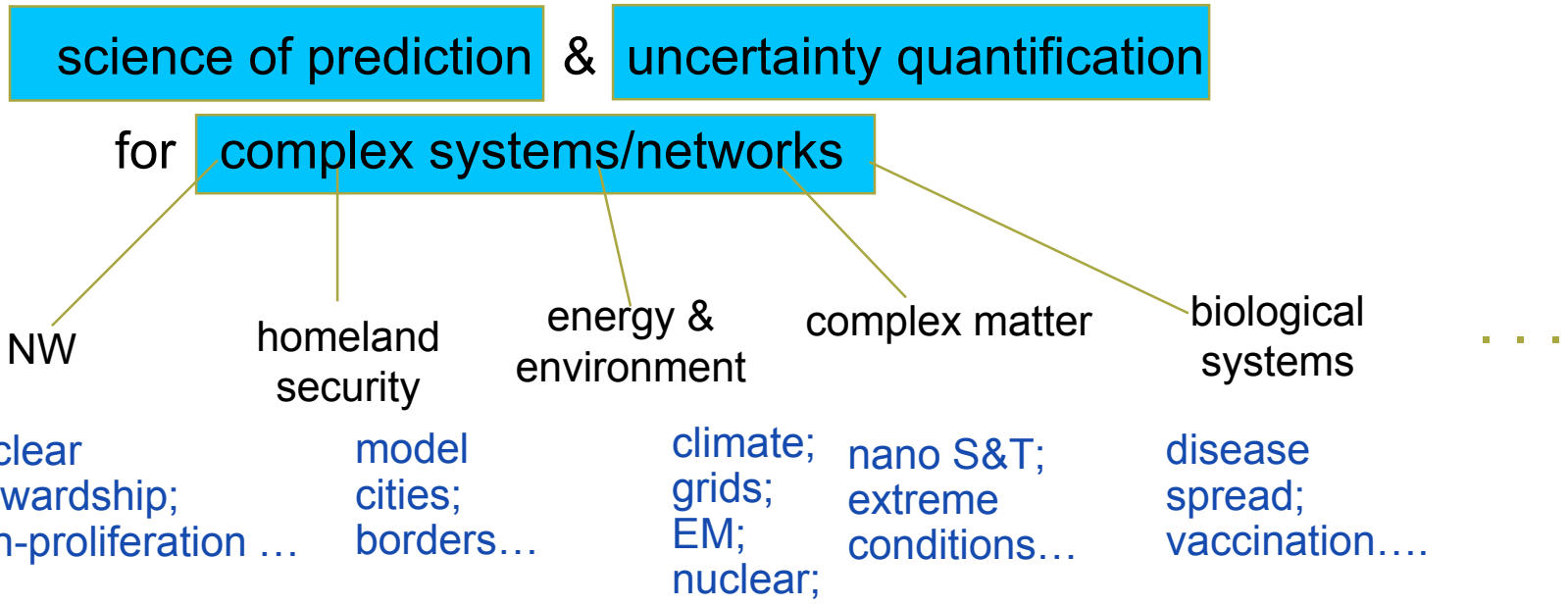
Protein Dynamics



Shocked Metals

The Promise and Challenge of Science (and Survival) in the 21st Century

- Isolating complicated phenomena to "understand" them necessary, but not sufficient



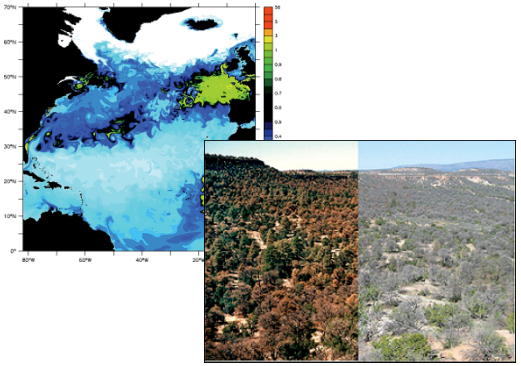
- Quantitative tools for decision makers/risk assessment
  - (coupled) socio, economic, humanities, physical sciences, …
  - from observation and validation to prediction and control

Energy-Climate Impacts Project (ECI) – Scientific Scope (Multi-Lab)

GHGIS – Measurements & Uncertainty Quantification

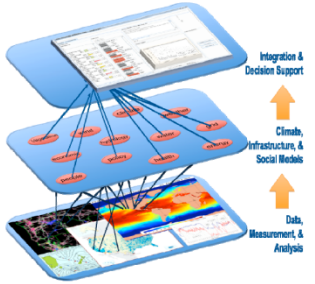
LANL ECI scientists contribute to the new GHGIS through estimating uncertainties, designing new instruments to measure GHGs, and using modeling to design the placement of new instruments.

Climate & Natural Systems Modeling



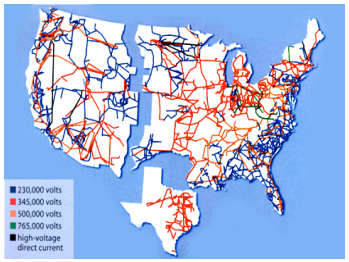
LANL ECI scientists participate in developing some of the most advanced climate models in the world: an ocean model, a sea ice model, physiology-based models for vegetation mortality, and a land ice model.

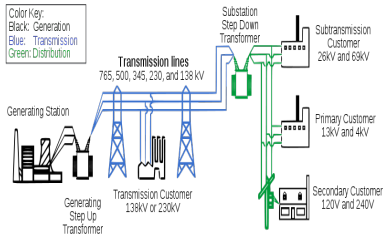
Social, Energy & Infrastructure Modeling for Climate Treaty support solutions



LANL ECI scientists can develop and apply Decision Support Systems to model the impacts of climate change and GHG emissions on regional and local scales and model its impacts on energy, social dynamics, and Infrastructure.

Smart Grid as a National Grand Challenge





R&D Problems for Smart Grids

A future grid, in which modern sensors, communication links, and computational power are used to improve efficiency, stability, and flexibility, has become known as the "smart grid."

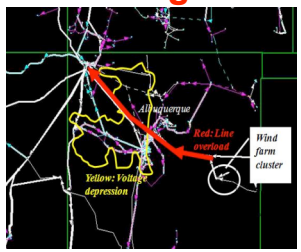
R&D Methodology: Road Map for Smart Grids

Our road map is driven by emerging technologies such as renewables, storage, and meters and accordingly specifies the technical challenges in *Grid Design*, *Grid Control* and *Grid Stability*.

All of the above require scientific advances in

- Analysis & Control
- Scalability/Reliability Mosaics
- State Estimation
- Data Aggregation & Assimilation
- Middleware for the Grid
- Modeling Consumer Response

Grid Designs

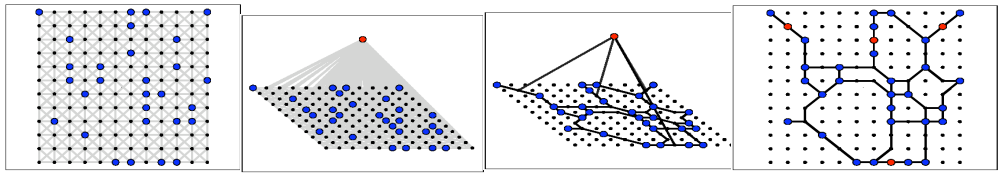


NREL solution included

- Cost dispatch only
- Power flows highly approximate
- Unstable solutions
- Intermittency in Renewables not accounted

Toole,Fair,Berscheid, Bent '09
go beyond NREL ``20% renewables ecorporated by 2030"

Generators – red dots
Loads – blue dots



original graph for generation placement

``master generator" connected to possible sites.

Resulting Sparse Network

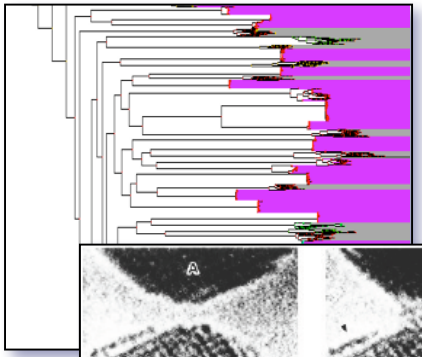
$$\begin{aligned} \text{minimize} \quad & \mathrm{Tr}(K(y)^{-1}W) + \textstyle\sum_{\ell \in G} c_\ell \left(\frac{y_\ell}{\hat{y}_\ell}\right)^\gamma \\ \text{subject to} \quad & 0 \le y_\ell \le \hat{y}_\ell \text{ for all } \ell \in G \end{aligned}$$

Johnson, Chertkov '09
Network Optimization

Impact to LANL, NNSA & the Nation

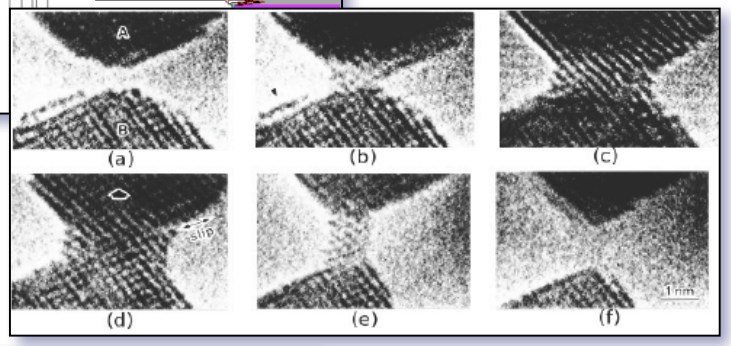
- **Reduce consumer energy costs**
- **Promote energy independence**
- **Support national renewable penetration goals**
- **Address strategic problems at the intersection of energy, climate, and infrastructure**
- **Support LANL's Energy Security Center and LANL's Information Science and Technology Center**

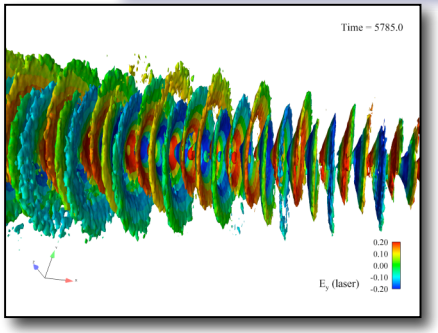
Los Alamos is committed to excellence in computer and computational sciences



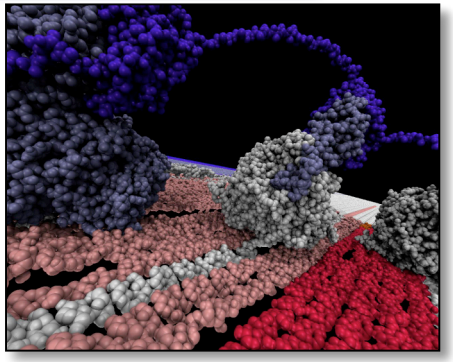
HIV epidemiology

Formation of nanomaterials





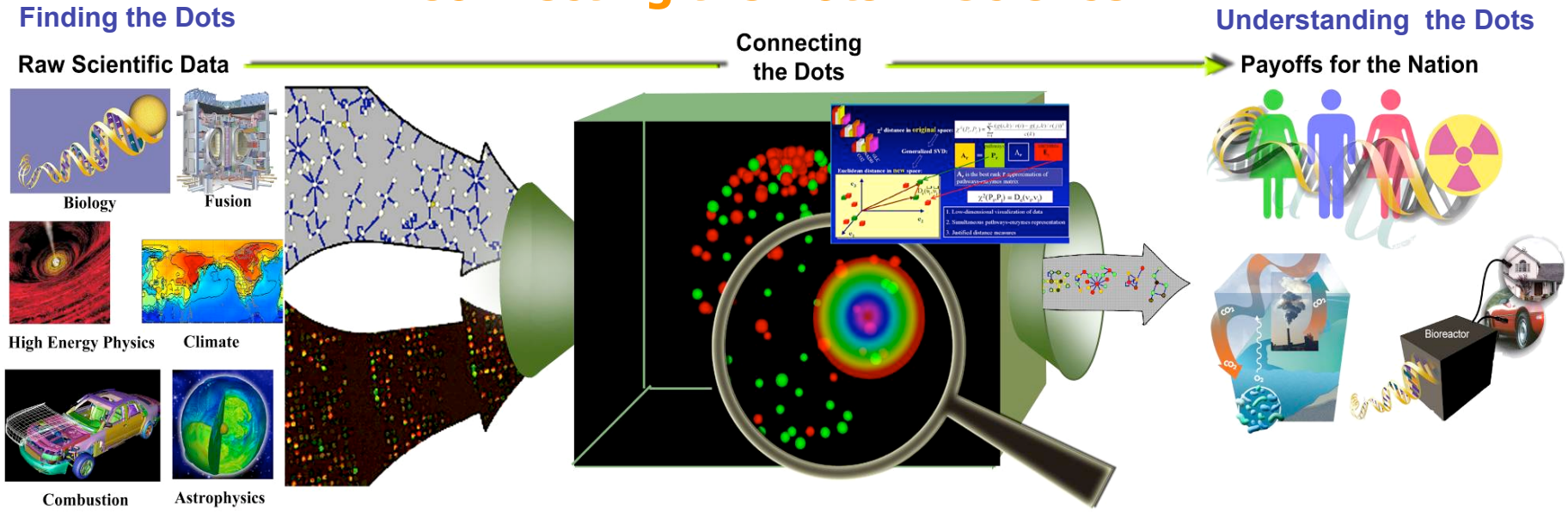
Laser plasma interactions



Breakdown of cellulose

- **Nuclear weapons program**
  - Support for enhanced Predictive/Control Capability
- **Open science**
  - Reliable and rich capability base for weapons
  - Enabling new science and mission frontiers
- **Institutional computing**
  - Supporting scientific innovation and technology development
  - Partnership with DOE-SC and ASC programs
- **Investing in the future**
  - Centers/Institutes
  - Exascale planning! (Joint DOE-SC/NNSA)
    - "Codesigning" applications, codes, architectures

Information Science & Technology is the Infrastructure for Connecting the Dots in Science



Sheer Volume of Data

Climate

Now: 20-40 Terabytes/year

5 years: 5-10 Petabytes/year

Fusion

Now: 100 Megabytes/15 min

5 years: 1000 Megabytes/2 min

Advanced Mathematics and Algorithms

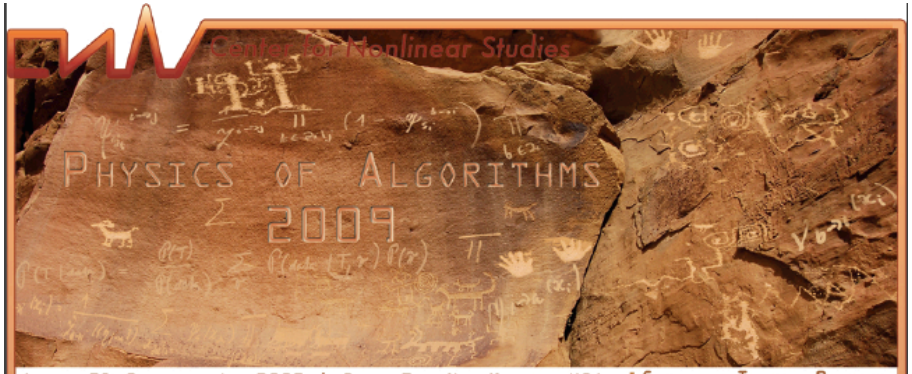
- Requires high-performance computing and advanced theory/modeling
- Huge dimensional space
- Combinatorial challenge
- Complicated by noisy data

Providing Predictive Understanding

- Produce hydrogen-based energy
- Stabilize carbon dioxide
- Clean and dispose toxic waste

c.f. Raymond L. Orbach, DOE Undersecretary for Science
2006 AAAS Annual Meeting

Office of Science
U.S. DEPARTMENT OF ENERGY
Los Alamos NATIONAL LABORATORY
EST. 1943



AUGUST 31-SEPTEMBER 4, 2009 | SANTA FE, NEW MEXICO, USA

http://cnls.lanl.gov/poa
conferences@cnls.lanl.gov

Optimization, inference and learning involve emerging computational problems in many areas of science and engineering. Typically stated in the framework of computer science and information theory, these problems are also linked to concepts and approaches native to statistical, mathematical and quantum physics.

This interdisciplinary field has seen a recent explosion of activity, resulting in new algorithms and new methods of analysis. Discrete computational challenges including constraint satisfaction and error correction have benefited from techniques and insights offered by statistical physics. Physics, at the same time, has been significantly enriched by approaches from discrete computation, such as convex optimization and message-passing algorithms.

Our workshop will bring together leading experts from physics, computer science, machine learning, operation research and information theory to discuss the current hot topics and new challenges in the intersection of these fields. Specific topics will include:

* GRAPHICAL MODELS
* STATISTICAL INFERENCE AND LEARNING
* MONTE CARLO ALGORITHMS
* BELIEF PROPAGATION AND MESSAGE PASSING ALGORITHMS
* SATISFIABILITY AND COMBINATORIAL OPTIMIZATION
* PHASE TRANSITIONS AND CAVITY APPROACH
* COMBINATORIAL APPROACHES (WALKS, LOOPS, ETC) RELEVANT TO THESE TOPICS

ORGANIZING COMMITTEE

Michael Chertkov, Los Alamos National Laboratory
Jason Johnson , Los Alamos National Laboratory
Allon Percus, Claremont Graduate University
Lenka Zdeborova, Los Alamos National Laboratory

Los Alamos NATIONAL LABORATORY EST.1943

This conference is:
Open to the Public with Registration

Center for Nonlinear Studies

CONFIRMED INVITED SPEAKERS

Stefan Boettcher
Emory
Vladimir Chernyak
Wayne State Univ.
Sue Coppersmith
Univ. of Wisconsin, Madison
David Gamarnik
Sloan School of Economics, MIT
Amir Globerson
Hebrew Univ.
Tom Hayes
Univ. of New Mexico
Koji Hukushima
Univ. of Tokyo
Shiro Ikeda
Inst. of Stat.Mechanics, Tokyo
Thomas Joerg
ENS, Paris
Werner Krauth
ENS, Paris
Florent Krzakala
ESPCI Paris
Martin Loebl
Charles Univ.
Jon Machta
Univ. of Massachusetts, Amherst
Alan Middleton
Univ. of Syracuse
Andrea Montanari
Stanford Univ.
Cris Moore
Univ. of New Mexico
Pablo Parrilo
EECS, MIT
Heiko Rieger
Univ. Saarlandes
Bart Selman
Cornell
Devavrat Shah
EECS, MIT
Alistair Sinclair
UC Berkeley
Sekhar Tatikonda
EE, Yale
Ricci-Tersenghi
La Sapienza, Rome
Massimo Vergassola
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Riccardo Zecchina
Politecnico di Torino